

# Identify More Pesticides Faster Using the Agilent High-Efficiency Source

The Agilent Pesticide DRS Screening GC/MSD Analyzer

## Application Note

Food Testing & Agriculture

### Authors

Melissa Churley and Bruce Quimby  
Agilent Technologies, Inc.

The Agilent Pesticide DRS Screening GC/MSD Analyzer, based on the Agilent 7890 GC and the Agilent 5977B GC/MSD, delivers fast screening and quantitation of large numbers of pesticides and endocrine disruptors in a single run. Deconvolution reporting software and a retention-time-locked database of pesticides and endocrine disruptors accelerates reporting and increases the number of targets screened. When configured with the 5977B GC/MSD and a high-efficiency source (HES), the analyzer identifies a greater number of pesticides while reducing analysis time.



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## Identify More Pesticides with the High-Efficiency Source

Routine analysis of residues in environmental and food samples requires confident identification and low-level detection along with fast reporting times. The GC/MSD pesticide analyzer addresses each of these needs through Deconvolution Reporting Software (DRS), which uses the NIST AMDIS program [1]. The Pesticides and Endocrine Disruptors database [2] accelerates reporting time, and increases the number of targets screened. In addition, proprietary capillary flow technology column backflush shortens cycle time, reduces chemical background, and optimizes uptime.

The 5977B GC/MSD and HES improve screening capability by increasing the number of ions created in the source and transferred into the quadrupole analyzer. More ions deliver more signal and, thus, better sensitivity. This increase in response translates into more targets found during the screening process with good library matches. Positive identification in food samples at 10 ng/g detection levels is now possible using the full-scan mode.

We demonstrated this in a DRS analysis of tomato extract that was spiked with over 200 pesticides at concentrations of 10 and 100 ng/g. This equates to injection of 10 and 100 pg of each pesticide, respectively. At the 10 ng/g level, 38 target compounds were identified using the HES as compared to none using the extractor source. Almost twice as many targets were identified at the 100 ng/g level (Table 1). Figure 1 shows an example AMDIS analysis for the target flusilazole, including raw and extracted spectra with library matching for the component.

## Conclusions

The Agilent Pesticide DRS Screening GC/MSD Analyzer delivers faster and more accurate screening of pesticides when configured with the Agilent 5977B GC/MSD and HES. When combined with Deconvolution Reporting Software, positive identification in full-scan mode for many targets in food at a concentration of 10 ng/g is possible.

Table 1. Number of AMDIS targets identified in tomato spiked at 10 and 100 ng/g using the extractor source (EXR) and HES (MMF = 80). The amount of pesticide injected was 10 and 100 pg, respectively. At the 10 ng/g level, 38 target compounds were identified using the HES as compared to zero using the extractor source. Almost twice as many targets were identified at the 100 ng/g level (Table 1). The NIST hit number breakdown (distribution) is given for categories 1st, 2nd, and  $\geq 3$  hit. Identified targets that were not spiked into tomato but had an AMDIS match score  $\geq 80$  and NIST hit no.  $\leq 3$  are also listed. Tuning conditions for each source are in parentheses.

	EXR (atune)		HES (autotune)	
	10 ng/g	100 ng/g	10 ng/g	100 ng/g
Number of targets with AMDIS score $\geq 80$	0	91	38	164
<b>Distribution of NIST hits</b>				
1st hit	0	63	26	144
2nd hit	0	12	7	14
$\geq 3$ rd hit	0	16	5	6
Not spiked, $\leq 3$ rd hit	2*	4**	2*	8***

\* Diethyl phthalate and benzophenone

\*\* Benzilamide, benzophenone, quintozone metabolite (pentachlorophenyl methyl sulfide), indoxacarb, and dioxacarb decomposition product [phenol, 2-(1,3-dioxolan-2-yl)-]

\*\*\* Diethyl phthalate, benzophenone, fonofos, phenol, phthalic acid, di(oct-3-yl) ester, phthalimide, quintozone metabolite (pentachlorophenyl methyl sulfide), indoxacarb, and dioxacarb decomposition product [phenol, 2-(1,3-dioxolan-2-yl)-]

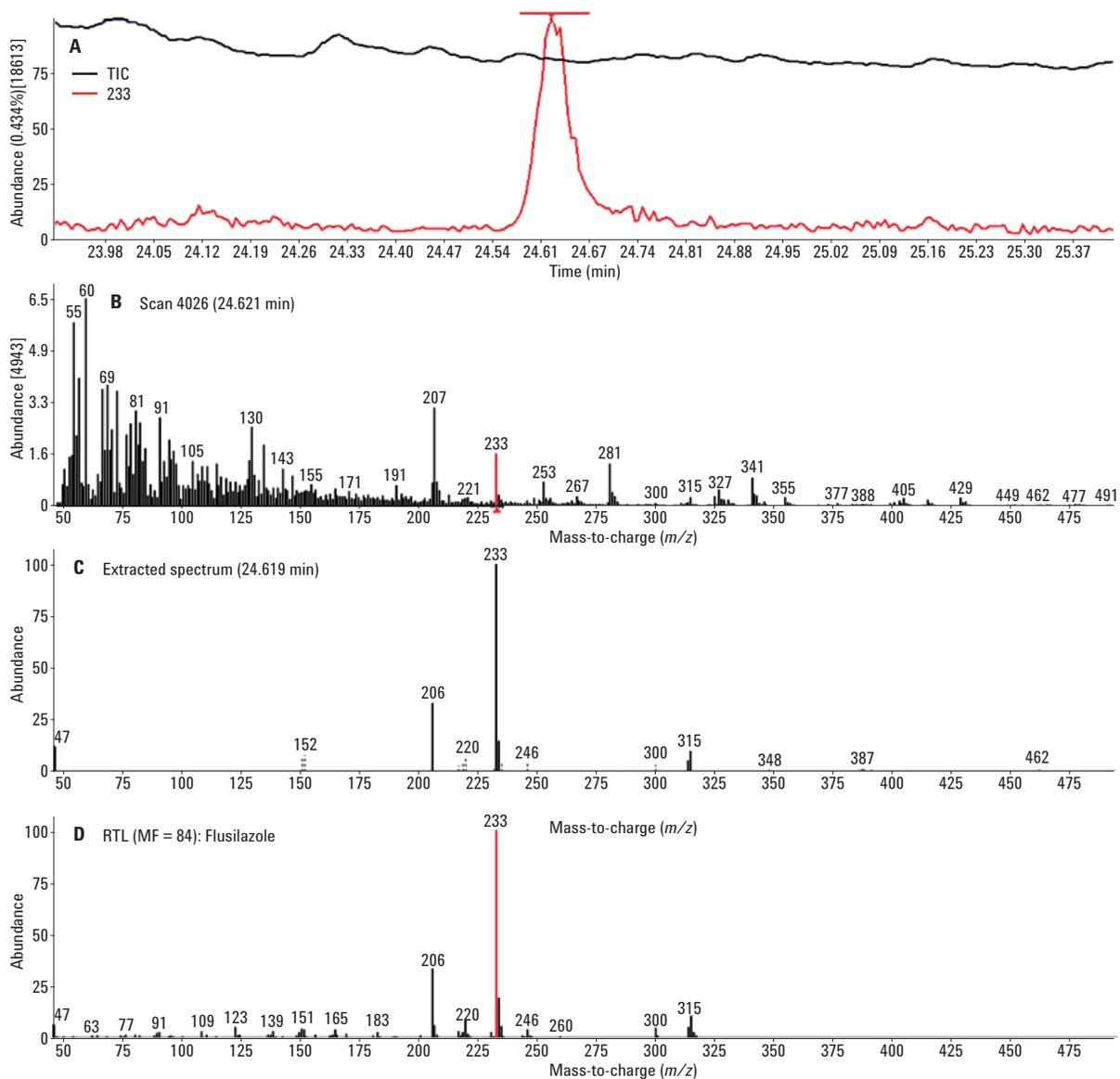


Figure 1. Analysis of 10 pg flusilazole in tomato using AMDIS. A) Overlay of extracted ion  $m/z$  233 (red) and TIC (black); B) raw spectrum; C) extracted spectrum for the component; D) library spectrum, AMDIS match factor = 84. The reported NIST reverse match score is 73.

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## References

1. Anon. NIST Standard Reference Database 1A, NIST/EPA/NIH Mass Spectral Library (NIST 14) and NIST Mass Spectral Search Program (Version 2.2), User's Guide. National Institute of Standards and Technology, U.S. Department of Commerce, Gaithersburg, MD, USA.  
<http://www.nist.gov/srd/upload/NIST1aVer22Man.pdf>
2. Wylie, P. L. *Screening for 926 Pesticides and Endocrine Disruptors by GC/MS with Deconvolution Reporting Software and a New Pesticide Library*; Application note, Agilent Technologies, Inc. Publication number 5989-5076EN, **2006**.

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